Electronic specific heat in the normal state of cuprate high-T_c superconductors

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By means of the composite operator method we calculate the specific heat of the 2D Hubbard model. Our results show that the model gives a detailed description of the experimental situation in the normal state of cuprate high T_c superconductors. The observed behavior is consistent with a Fermi liquid picture where the unusual properties are described in terms of the van Hove scenario. There is experimental evidence, based on the data for the spin magnetic susceptibility and specific heat, that this scenario is related to the overdoped region where superconductivity is depressed.

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A remarkable property of cuprate materials is the presence of a van Hove singularity (vHs) near the Fermi level in the hole-doped compounds [1]. Based on this experimental result a van Hove scenario for high T_c superconductors has been proposed [2-4]. Now, there are two quantities, the coefficient of the electronic specific heat $\gamma = C/T$ and the spin magnetic susceptibility $\chi(\mathbf{k},\omega)$, which are directly connected to the density of states (DOS) and can give important information on the role played by the vHs. In our previous articles [5-7] we have presented a series of theoretical results where we showed that the single-band 2D Hubbard model can give a detailed description of the normal state magnetic properties observed in high T_c materials. In particular, the picture that emerges from our studies [6,7] of the magnetic susceptibility is consistent with the van Hove scenario, where the unusual observed behavior is explained by the fact that upon doping the Fermi level approaches the vHs.

In this Letter we shall examine the electronic specific heat and we will show that also in this case the Hubbard model is a realistic model capable to describe the thermodynamic properties of the oxides in the framework of the van Hove scenario.

The electronic specific heat $C(T)$ of cuprate high T_c superconductors has been measured. In particular $C(T)$ of $La_{2-x}Sr_xCuO_4$ [8] has been studied for $0.03 < x < 0.44$ in the range of temperatures between 1.5 and $300K$, and of $YBa_2Cu_3O_{6+y}$ [9] for $0.16 \leq y \leq 0.97$ between 1.8 and $300K$. In Ref. 10 the electronic specific heat of $La_{2-x}Ba_xCuO_4$ has been measured in the range $0.025 < x < 0.25$ at low temperatures. From these experiments the following behavior has been observed for the coefficient $\gamma = C/T$ of the normal state specific heat:

a. for fixed temperature, $\gamma(x,T)$ increases with doping;

(a1) in the case of $La_{2-x}Sr_xCuO_4$, $\gamma(x,T)$ exhibits a rather sharp maximum at $x \approx 0.25$ (near the doping where superconductivity disappears), then starts to decrease; for $La_{2-x}Ba_xCuO_4$ a maximum has been observed at $x \approx 0.22$;

(a2) in the case of $YBa_2Cu_3O_{6+y}$, $\gamma(x,T)$ increases smoothly to a plateau or two broad maxima, situated at $y \approx 0.6$ and $y \approx 0.9$, respectively;

b. for fixed doping, $\gamma(x,T)$ as a function of temperature exhibits a broad peak moving to lower temperatures with increasing the dopant concentration;

c. further increasing y, the T dependence weakens and in the region of high doping no increase is observed. For $YBa_2Cu_3O_{6+y}$, no substantial increase is observed for $y > 0.8$.

To interpret these results, let us recall that the coefficient of the electronic specific heat $\gamma = C/T$ can be expressed as

$$\gamma(T) = \frac{1}{T}\frac{d}{dT}\int_{-\infty}^{+\infty} d\omega N(\omega) f(\omega)\omega \qquad (1)$$

where $N(\omega)$ is the density of states and $f(\omega)$ is the Fermi distribution function. This expression explicitly shows that $\gamma(T)$ reflects thermal average of the density of states. The presence of a maximum (or two maxima) for a critical doping is related to the fact that the Fermi energy lies on the vHs. Interpretation of the experimental results obtained in Ref. 9 for $YBa_2Cu_3O_{6+y}$ in terms of a sharp feature in the density of states, consistent with ARPES experiments [1], was firstly advanced in Refs. 11 and 12. The consistence of thermodynamic data with the presence of a vHs near the Fermi level was shown in Ref. 13 by considering a p-d like-model in the framework of slave-boson mean-field theory in the limit of large U.

In this Letter we shall consider the two-dimensional single-band Hubbard model by means of the Composite Operator Method (COM) [14,15]. In a standard notation this model is described by the Hamiltonian

$$H = \sum_{ij} t_{ij} c^{\dagger}(i) \cdot c(j) + U \sum_{i} n_{\uparrow}(i) n_{\downarrow}(i) - \mu \sum_{i} c^{\dagger}(i) \cdot c(i) \quad (2)$$

To discuss the specific heat it is useful at first to consider the non interacting [i.e. U=0] Hubbard model. In Fig. 1 we report $\gamma(x,T)$ as a function of T for various values of the filling. We see that at half-filling $\gamma(x,T)$ diverges as $T \to 0$; this is an effect of the vHs. When doping is introduced the Fermi energy moves away from the vHs and the peak exhibited by $\gamma(x,T)$ moves away from $T = 0$. $\gamma(x,T)$ firstly increases as a function of T, exhibits a maximum at a certain temperature T_m and then decreases. The temperature behavior of $\gamma(x,T)$ is similar to the one exhibited by the static uniform spin magnetic susceptibility $\chi_0(x,T)$ [16,5]. When we move away from half-filling the value of T_m increases up to a certain doping, then decreases. For a fixed temperature $\gamma(x,T)$ exhibits a doping dependence of different behaviour from the one presented by $\chi_0(x,T)$. At $T = 0K$ $\gamma(x,T)$ diverges at $n = 1$ and then decreases by lowering n. At nonzero temperature the peak splits in two peaks, symmetric with respect to $n = 1$ where it has a minimum. This is shown in Fig. 2, where $\gamma(x,T)$ is reported as a function of the filling at various temperatures. The shift of the two peaks with respect to n=1 increases by increasing T.

When we consider the interacting case [i.e. $U \neq 0$], the specific heat in COM is calculated by means of the following expression

$$C(T) = \frac{d}{dT} \int \frac{d^2k}{(2\pi)^2} \{A_1(\mathbf{k}) f[E_1(\mathbf{k})] E_1(\mathbf{k}) + A_2(\mathbf{k}) f[E_2(\mathbf{k})] E_2(\mathbf{k})\} \quad (3)$$

where $E_1(\mathbf{k})$ and $E_2(\mathbf{k})$ are the energy spectra; $A_1(\mathbf{k})$ and $A_2(\mathbf{k})$ are some weight functions, calculated from the spectral intensities of the Green's function, defined by $G(\mathbf{k},\omega) = \langle T[\psi(i)\psi^{\dagger}(j)]\rangle_{F.T}$, where $\psi(i)$ is the doublet composite operator

$$\psi(i) = \begin{pmatrix} \xi(i) \\ \eta(i) \end{pmatrix} \quad (4)$$

with

$$\xi_{\sigma}(i) = c_{\sigma}(i)[1 - n_{-\sigma}(i)] \quad (5)$$

$$\eta_{\sigma}(i) = c_{\sigma}(i) n_{-\sigma}(i) \quad (6)$$

By means of the equation of motion and by considering the static approximation, where finite lifetime effects are neglected, the Green's function $G(\mathbf{k},\omega)$ can be computed in the course of a fully self-consistent calculation where no adjustable parameters are considered [14]. In Fig. 3 we present the linear coefficient $\gamma(x,T) = C(x,t)/T$ as a function of the doping for various temperatures. As general behavior we see that by increasing the doping $\gamma(x,T)$ increases up to a certain doping and then decreases. The nature of the peak is again due to the fact that the Fermi energy crosses the vHs for a certain critical value of x. However, differently from the case of spin magnetic susceptibility, the peak position of $\gamma(x,T)$ depends on the temperature. In the limit of zero temperature a sharp peak is exactly located at $x = x_c$. By increasing the temperature the peak moves away from x_c and broadens in two peaks. The situation is similar to what can be calculated for the free case and illustrated in Figs. 1 and 2. The behavior described in Fig. 3 well reproduces the experimental situation. As reported in Refs. 8 and 10, peaks in the normal state linear coefficient are observed in $La_{2-x}Sr_xCuO_4$ and in $La_{2-x}Ba_xCuO_4$; the position of the peaks is close to the doping where superconducting is suppressed, but there is a small shifting, due to the temperature effect. In the case of $YBa_2Cu_3O_{6+y}$, the experimental results reported in Ref. 9 are for the higher temperature $T = 280K$; $\gamma(x,T)$ increases with doping and presents two broad maxima in the region of high doping. In Figs. 4 and 5 we present the linear coefficient $\gamma(x,T)$ as a function of the temperature for values of the filling $x > x_c$ and $x < x_c$, respectively. At $x = x_c$ we see that $\gamma(x,T)$ diverges as $T \to 0$; this is an effect of the vHs. When $x \neq x_c$ the Fermi energy moves away from the vHs and the peak exhibited by $\gamma(x,T)$ moves away from $T = 0$. $\gamma(x,T)$ firstly increases as a function of T, exhibits a maximum at a certain temperature T_m and then decreases. The behavior of $\gamma(x,T)$, when reported versus temperature, is similar to the one exhibited by $\chi_0(T)$ [16,5]. As shown in Fig. 5, when the doping is increased the value of T_m moves to lower temperatures. This behavior qualitatively agrees with the experimental situation reported in Ref. 9. The fact that for $YBa_2Cu_3O_{6+y}$ $\gamma(x,T)$ is always a decreasing function of T when $y > 0.8$ indicates a low value of T_m, below the critical superconducting temperature, which is the case near the critical doping.

The main results obtained in this Letter can be so summarized. Experimental data for the linear coefficient of the specific heat γ in the normal state of hole-doped cuprates show the existence of doping where the density of states is enhanced, revealing the nearness of the Fermi level to the vHs. This is in agreement with the ARPES experiments. The critical doping where the Fermi level crosses the vHs is very close to the critical doping where the superconducting phase is suppressed.

In the single-band Hubbard model the interaction has mainly two effects. From one hand the critical doping is shifted from $x = 0$ to some critical x_c. The value of x_c depends on the ratio U/t and varies between 0 and 1/3 [5]. For $U/t = 4$ it is found that $x_c = 0.27$, very close to the experimental value observed in $La_{2-x}Sr_xCuO_4$ [16]. The shifting of the Fermi energy with respect to the

vHs by varying the doping explains and well reproduces the unusual normal state behavior of $La_{2-x}Sr_xCuO_4$ in the normal state of hole-doped cuprates. The other role played by the interaction is a band structure effect which creates an asymmetric double peak in the specific heat, as shown in Fig. 5. The picture of an ordinary Fermi liquid which emerges from our calculations agrees with the experimental situation in $YBa_2Cu_3O_{6+y}$ [17], where no separation of spin and charge degrees of freedom has been observed. In the context of the Hubbard model a van Hove scenario well describes some of the unusual properties observed in the normal state; there is experimental evidence, based on the data for susceptibility [16] and specific heat [8,10], that this scenario is related to the overdoped region and not to the optimal doping.

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FIG. 1. The linear coefficient of the normal state specific heat $\gamma = C/T$ of the non interacting 2D Hubbard model is reported as a function of the temperature for various values of the particle density. The temperature is expressed in units of the hopping parameter t.

FIG. 2. γ of the non interacting 2D Hubbard model is reported as a function of the filling for various values of the temperature.

FIG. 3. γ of the interacting 2D Hubbard model is reported as a function of the doping parameter $x = 1 - n$ for various values of the temperature and $U/t = 4$.

FIG. 4. γ of the interacting 2D Hubbard model is reported as a function of the temperature for various values of the doping $x > x_c$ and $U/t = 4$.

FIG. 5. Same as in Fig. 4, but for $x < x_c$.

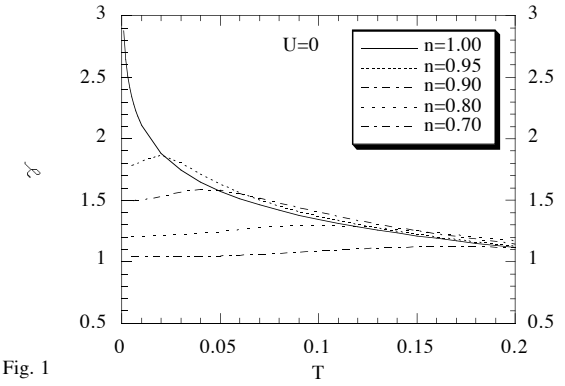

Fig. 1

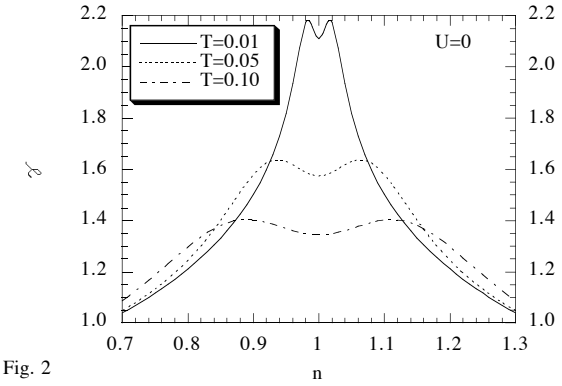

Fig. 2

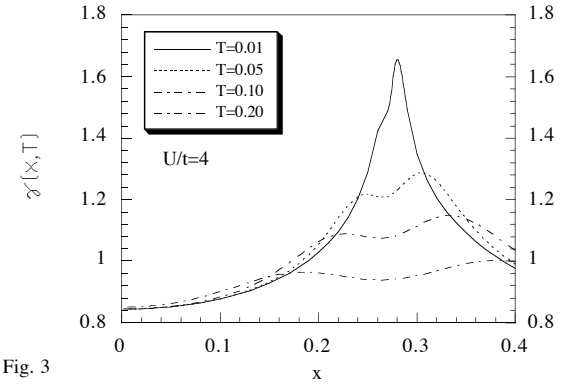

Fig. 3

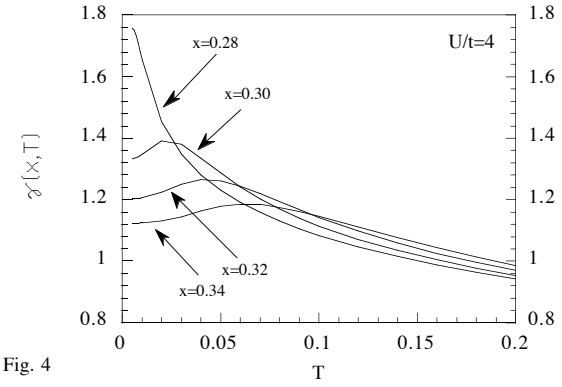

Fig. 4

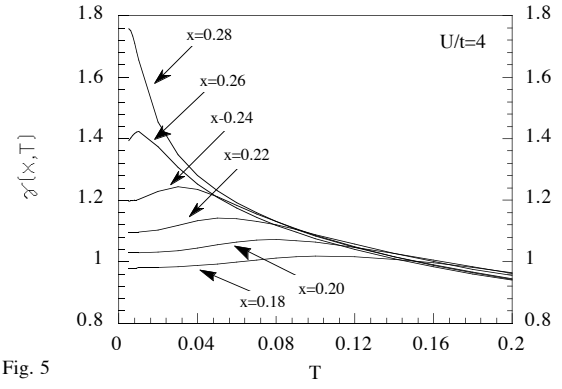

Fig. 5